

## REPORT DOCUMENTATION PAGE

Form Approved  
OMB No. 0704-0188

1a. REPORT SECURITY CLASSIFICATION Unclassified		1b. RESTRICTIVE MARKINGS	
2a. SECURITY CLASSIFICATION AUTHORITY DTIC SELECTED		3. DISTRIBUTION/AVAILABILITY OF REPORT Approved for public release; distribution is unlimited	
2b. DECLASSIFICATION/DOWNGRADING SCHEDULE 2012 01 01 1995		4. PERFORMING ORGANIZATION REPORT NUMBER(S) F	
5a. NAME OF PERFORMING ORGANIZATION Rensselaer Polytechnic Institute		5b. OFFICE SYMBOL (if applicable) Chemical Eng.	
6a. ADDRESS (City, State, and ZIP Code) Troy, NY 12180-3590		7a. NAME OF MONITORING ORGANIZATION ONR, Code 333	
6b. ADDRESS (City, State, and ZIP Code) 800 North Quincy St., Room 504 Arlington, VA 22217		7b. ADDRESS (City, State, and ZIP Code) 800 North Quincy St., Room 504 Arlington, VA 22217	
8a. NAME OF FUNDING/SPONSORING ORGANIZATION ONR, Code 333		8b. OFFICE SYMBOL (if applicable)	
9. PROCUREMENT INSTRUMENT IDENTIFICATION NUMBER N-00014-94-1-0097		10. SOURCE OF FUNDING NUMBERS	
3c. ADDRESS (City, State, and ZIP Code) 800 North Quincy St., Room 504 Arlington, VA 22217		PROGRAM ELEMENT NO. 601153N	PROJECT NO. 02402
		TASK NO. 010	WORK UNIT ACCESSION NO.
11. TITLE (Include Security Classification) Gas-Phase Kinetics Measurements for Underwater Explosives			
12. PERSONAL AUTHOR(S) Arthur Fontijn			
13a. TYPE OF REPORT Annual	13b. TIME COVERED FROM 10/15/94 TO 10/14/95	14. DATE OF REPORT (Year, Month, Day) 95/10/9	15. PAGE COUNT 4
16. SUPPLEMENTARY NOTATION			
17. COSATI CODES		18. SUBJECT TERMS (Continue on reverse if necessary and identify by block number)	
FIELD	GROUP	SUB-GROUP	
			Explosives
			Reaction Kinetics
			Fluoro-Nitramino
			BO
			Boron
19. ABSTRACT (Continue on reverse if necessary and identify by block number)			
<p>To aid in the development of boron-enhanced fluoronitramino explosives, the kinetics of individual reactions are measured over wide temperature ranges. Using the HTFFR technique it was established that, for <math>BO + HCl \rightarrow OBCl + H</math>, <math>k(300-760\text{ K}) = 5.7 \times 10^{-13} \exp(-1437\text{ K/T}) \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}</math>. Currently this determination, and HTFFR results on the BO reactions with <math>O_2</math>, <math>CO_2</math> and <math>N_2O</math>, are being checked with an MHTP reactor.</p>			
20. DISTRIBUTION/AVAILABILITY OF ABSTRACT <input checked="" type="checkbox"/> UNCLASSIFIED/UNLIMITED <input type="checkbox"/> SAME AS RPT. <input type="checkbox"/> DTIC USERS		21. ABSTRACT SECURITY CLASSIFICATION Unclassified	
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19951018 098

DTIC QUALITY INSPECTED 8

## PROGRESS

Our goals are:

- (i) to make accurate measurements, over wide temperature ranges, of rate coefficients for boron combustion in C/H/N/O/F environments, of importance to the development of new underwater explosives, and
- (ii) to use the measurements to obtain a further understanding, to allow predictions for additional reactions occurring with such explosives.

Our efforts this past year have concentrated on completing the series of experiments on BO reactions in a high-temperature fast-flow reactor (HTFFR) and preliminary experiments on reactions of this species in a metals high-temperature photochemistry (MHTP) reactor. Additionally, a series of experiments was undertaken to test the ability of our reactors to withstand HF at high temperatures, in preparation for studies with this reactant; no problems were encountered. However, it was found desirable to protect the vacuum pump with a CaO trap, and for work with BF and BF<sub>3</sub>, additionally with an activated carbon trap.

Previously, in the HTFFR study of the BO + O<sub>2</sub> reaction, unusually wide scatter in the rate coefficients was encountered.<sup>1</sup> As earlier work in a reactor, fashioned after our MHTP reactors, had not shown such scatter,<sup>2</sup> this suggested to do further work on this reaction using that approach, following some further HTFFR studies. The additional BO reactions thus studied this year were BO + HCl and N<sub>2</sub>O. Of these the first did not show appreciable scatter, but with the second the scatter was again unsatisfactorily high. We obtained, in units of cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup>,

- (1)  $\text{BO} + \text{HCl} \rightarrow \text{OBCl} + \text{H} \quad \Delta H = -5.7 \pm 37 \text{ kJ mol}^{-1}$   
 $k_1 (300\text{-}760 \text{ K}) = 5.7 \times 10^{-13} \exp(-1437 \text{ K/T})$
- (2)  $\text{BO} + \text{N}_2\text{O} \rightarrow \text{BO}_2 + \text{N}_2 \quad \Delta H = -367 \text{ kJ mol}^{-1}$   
 $k_2 (300\text{-}1000 \text{ K}) = 3 \times 10^{-13} \exp(-1310 \text{ K/T})$

where our confidence is considerably higher in the first than in the second result. Checks on both reactions will be conducted in the HTP reactor this coming year. Presumably, less effort there will have to be expended on the first than on the second reaction.

Currently, we are engaged in re-measuring the reaction

- (3)  $\text{BO} + \text{O}_2 \rightarrow \text{BO}_2 + \text{O}$

in the HTP facility. After that, and extending into the proposed contract extension period, we will check the HTFFR result<sup>1</sup> that

- (4)  $\text{BO} + \text{CO}_2 \rightarrow \text{BO}_2 + \text{CO}$

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has rate coefficients of less  $1 \times 10^{-15}$  over the 780-1200 K temperature range. This is our result that has thus far the most direct impact on current models,<sup>3</sup> as it is some three orders of magnitudes slower than guessed in those models.

The proven methods to produce BO in the HTP reactor is the photolysis of  $\text{BCl}_2(\text{OCH}_3)$ , which appears to be good up to around 1000 K.<sup>2,4</sup> We are also considering another method referenced in the same articles. That method is photolysis of a boron compound such as  $\text{BCl}_3$  to produce B atoms, followed by BO production from their reaction with an oxidant such as  $\text{O}_2$ . It has been observed to suffer from interference from vibrational relaxation, but would have the advantage of allowing work at much higher temperatures, at least 1400 to 1500 K. The problem in previous work with this production method was that vibrational relaxation occurred on the same time scale as the reaction, when narrow beam laser-induced fluorescence was used. However, by using a cw flowlamp, or an expanded laser beam, the time scale of MHTP experiments can be increased by several orders of magnitude,<sup>5</sup> and a vibrational relaxation agent, such as  $\text{SF}_6$ , may help further.

### PLANS

Our reaction selection will continue<sup>1</sup> to be based on the Aerodyne-Princeton modeling work<sup>3</sup> and checks thereof. As a result of discussions at the June 1995 Boron Combustion Workshop, on the work of Drs. Mike Page and Maribel Soto, we have now removed  $\text{BF} + \text{HF}$  from the list, while  $\text{BF} + \text{H}_2\text{O}$  has increased in importance. Thus in addition to reactions (1) - (4) above, the list for study, discussed last year, now looks as follows, in the approximate sequence planned for study:

$\text{BO} + \text{N}_2\text{O}$ ,  $\text{HF}$ ,  $\text{BF}_3$ ,  $\text{H}_2\text{O}$

$\text{BF} + \text{H}_2\text{O}$ ,  $\text{O}_2$ ,  $\text{BF}_3$ ,

$\text{BO}_2 + \text{N}_2\text{O}$

$\text{F} + \text{H}_2\text{O}$

### PARTICIPANTS AND CONTACTS

The experimental work has been performed by G.T. Dalakos with help from D.P. Belyung. In addition to these two students, W.F. Flaherty, our group technician, has participated. We thank Dr. R.A. Yetter for several informative discussions.

### PUBLICATIONS AND AWARDS

None this year.

## References

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